

2-benzyl-6-methylpyrazine

Inchi:	InChI=1S/C12H12N2/c1-10-8-13-9-12(14-10)7-11-5-3-2-4-6-11/h2-6,8-9H,7H2,1H3
InchiKey:	FCJOWQOYTARQAR-UHFFFAOYSA-N
Formula:	C12H12N2
SMILES:	Cc1cncc(Cc2ccccc2)n1
Mol. weight [g/mol]:	184.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	2.376		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
ripol	2325.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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